**2nd quantization**

As we could see in the preceding files, it becomes arduous to keep track of the symmetrization requirements of the N-particle wavefunction when dealing with identical particles. As a consequence, people began looking for a more concise formulation of quantum mechanics that took into account the symmetrization requirements from the beginning. The technique developed is called, rather misleadingly, second quantization. This is presumably because the Heisenberg time-development equation for some of the creation/annihilation operators looks similar to the Schrodinger equation, and so it ‘looks’ like the wavefunction itself has been quantized. But this isn’t what’s going on. And this formalism doesn’t have any more ‘quantization’ in it than any other part of Quantum Mechanics does. Any way, the main ideas are these.

**Postulate 1: Fock Space**

Suppose we have N particles. Then the HS on which the wavefunction describing these N particles exists is:



And the state of the system can be described by specifying the location/spin of each particle, i.e., by picking out a vector in each of the direct product Hilbert spaces. In other words a possible wavevector would be:



But this is ignoring symmetrization requirements. And in reality, this isn’t possible state of the system. Rather, such a basis state would be:



where ε{123…N} is the symmetrization factor which is 1 for bosons, or the anti-symmetric tensor for fermions. So the lesson is that not all the many body basis states that one can construct in the HS are actual states that can *physically* exist. So the idea is to prune off all of the unphysical basis states from the HS, and what is left is called Fock Space (FS). We can specify all of the basis states in the FS, i.e., simply by specifying the occupation number of all of the allowed single particle states. So we would write:



where ni is the number of particles in state *i*. State *i* would be |**r**imsi> in the above example. Clearly in this case, *i* is a continuous index that runs over all positions and spin orientations. In 2nd quantization notation, we would, using the position basis as above, denote states like this:



where we make a slot for each position in 3D space and spin orientation possible (obviously this isn’t literally possible since there are a continuously infinite number of possible configurations but this is the idea). The n’s are the occupation numbers for each position/spin. These occupation numbers can be between 0 and ∞ for boson systems. But they can only be 0 or 1 for fermion systems (due to Pauli-exclusion principle).

Either way we denote the state, either in HS or FS, more general states can be built up by making linear combinations of these basis states.

One final note. We do not have to index the possible states using the position basis. We can use any basis we choose – the momentum basis, the energy basis (of some Hamiltonian), etc. We just need some basis that spans the single particle HS.

**Example**

Suppose we have two electrons with in a 1D infinite box with length *a*. What are the physical states in the HS? What is the wavevector for two electrons – one in the n = 1 state spin up, and one in the n = 3 state spin down? How are these denoted in FS?

Let |ψ> = |nms> represent the one particle states. These are the familiar:



Then the physical two-particle states are:



The wavevector for the particular configuration mentioned would be:



In the FS, these two particle states would be represented in the following notation. We would index each of the one particle states with a slot, and then fill in the occupation number of each state. So the allowed states would look something like this below.



Each occupation number can be either 0 or 1 (no more than 1 due to the Pauli-exclusion principle), and the sum of all the occupation numbers must be 2 since we have two particles. For the particular configuration mentioned, the wavevector would be:



Obviously, with an infinite number of possible states, this isn’t a concise way to write a wavefunction, but we rarely attempt to write the wavefunction this way when using 2nd quantization so its OK.

**Example**

Suppose we have some operator K whose basis kets we use to span the single particle HS. And let the eigenkets of K be denoted |kn>. How would we write the bosonic state

|ψ> = |010200…> in the HS?

We would write it as:



**Postulate 2: Creation/Annihilation operators**

With the basis kets of the FS, we can define operators in the FS, since operators are fundamentally just mappings between basis kets. Suppose we use the one particle eigenbasis of the operator , with eigenvalues ai and single particle states |ai> to index the possible states in the FS. The basis states in the FS are then indexed as:



Now let’s introduce the annihilation operator i and creation operator i† (gonna be leaving off the hats often times, though). When acting on a state |ψ>, these operators produce a new state with one less and one more particle respectively in the state |ai>. There are pre-factors involved though, and the mathematical definition for bosons is:



You’ll note this is the same as harmonic oscillator factors. And for fermions we have:



Let’s consider the commutation relations between these operators for bosons…



If consider anticommutator of fermionic operators,



And so we have (didn’t really prove the j ≠ i cases, but you can):



as well as:

 

Might note that the fermionic anti-commutation relations themselves prevent occupation numbers greater than 1. For instance,



We can change the single particle basis parameterizing our system if we wish. Suppose we want to describe the system in the single particle basis, |bi >, then bi, bi† would be our annihilation/creation operators. And we’d like to express bi and bi† in terms of ai, ai†:



so we must have:



and



**Position and ‘momentum’ creation/annihilation operators on a lattice**

Consider a lattice, and a set of basis functions defined on each primitive cell. Well actually, we’ll consider just one basis function on the primitive cell (though with two possible spin orientations). So our set of basis function is: |Rσ>, where R can be any lattice site. And now we’ll define creation/annihilation operators that add/subtract a particle to the primitive cell at **R**. For instance, ψ**R** would be the annihilation operator at site **R.** And let the lattice spacing be ax, ay, az, in the respective dimensions. We’d like to go to Fourier space, etc. So then we’d have,



where,



We also have the completeness relations



**3D finite continuous volume with periodic boundary conditions**

In this case, the lattice spacing, a, goes to 0 and R assumes a continuously infinite array of values. So we’ll relabel **R** → **r**. And **k** can assume an infinite set of denumerable values.



and so our expressions would transform to:



Then we usually multiply ψk by 1/√a3, and ck by √a3, to make them symmetrically defined, and have,



the  are conventional. This corresponds well to the usual convention as:



And the completeness relations are:



Note that the commutation relations for the ψ’s will be, presuming fermions for the sake of discussion:



So moral of story is that continuum operators obey commutation relations analogous to the discrete ones – just replace Kronecker δ with Dirac δ.

**3D infinite continuous volume**

Now we take L itself to infinity. This transforms the discrete sums over k to integrals over k, with 2π/L being the spacing between k values. Using the conventional basis transformation stuff discussed above, we’ll have:



where ψσ(x) annihilates a particle at position x and spin σ, and ckσ annihilates a particle with momentum k, and spin σ. The completeness relations then become



**Fourier transform relations**

Finally, since Fourier transforms are going to be encountered so much, it is helpful to recognize that





where



**Wavefunctions**

We can determine wavefunctions just like we did before, as overlaps between states. Say we have a single particle in state |ks>. What is its wavefunction? Note ε = ±1 for Fermions/Bosons.



Now let us have two particles with momenta/spin k1s1, and k2s2. What is their wavefunction? We form,



Now we need to commute the annihilation operators to the other side. We’ll get (ε = ±1 for fermions/bosons), disregarding terms that annihilate the vacuum:



which is indeed the symmetrized wavefunction. I think. Well, so:



Well these are technically the same, since they’re off by overall ε, which doesn’t matter: phase factors don’t matter. A little more concretely, the wavefunction would look like,



and if s1, s2 were spin up, spin down. Then this would look like,



**Representation of operators in FS**

In many body problems one frequently encounters operators that are the sum of one-particle operators. For instance, in a system of N non-interacting particles situated in a potential V(r), the total momentum P, and energy H, operators are:



Note that these definitions also imply that the multi-particle operator:



can be written in terms of creation and annihilation operators defined over its one particle eigenbasis states as:



We can also change to a one-particle basis of states that aren’t eigenkets of the one particle operator V1(1). Suppose we change to the eigenbasis of the one particle operator A, with eigenvalues, ai. Let ai, ai† be the annihilation and creation operators that subtract and add one particle to the system with eigenvalue ai. Then we can write that V is equal to:



So this gives us the general formula for writing an additive one-particle operator in terms of creation and annihilation operators of a particular basis in Fock space.



Two particle operators can be calculated roughly in the following manner. Let



Choose FS basis to be V2 eigenvectors – this would be the position basis. Then,



(the second term is including interactions between particles in the same position) Putting this in terms of the creation/annihilation operators we have (|b> would be the position basis, but leaving as more general):



and converting to an arbitrary basis, |ai> we have,



And so,



In the sense that the quantum numbers are read inward to outward. You should think of <i|V|j> as something like the energy cost of going from the state |j> to the state |i>. And so <i|V|i> would just be the energy content of |i>. Similarly, <ij|υ|kℓ> is the energy cost of going from the state |kℓ> to the state |ji>. And likewise, <ji|υ|ij> would just be the energy content of the state |ij>. This interpretation enables us to construct these models more heuristically, especially when the allowed states |i> are heuristically constructed. And to construct H, we would just sum up the energy transfers between all possible pairs of states.

**Postulate 3: Time development**

The usual time-development formulas carry over. We have of course,



and,



as well as:



Let’s consider the special case of a time-independent H, and consider the time-development an annihilation operator. It follows from, ignoring h’s…



Let’s specialize to the particular Hamiltonian,



So we just compute this commutator to obtain the equation of motion for the operator (subscript H on commutator means to take time development of the commutator when done).



The last two are the same, and so we just have:



So it is just like we had multiplied H by the inverse of the first creation operator, in the matrix sense. Time development is also determinable from the Baker – Hausdorf formula – presuming time-independent H below:



Just realized I presumed they were bosons. What if they’re fermions? Let’s do just a single particle H.



Then we have:



So same so far. OK let’s do the V part too.



Last two guys cancel of course. And then maybe switching the pj indices of the first guy’s bra <| costs us a minus sign (because of anti-symmetrization, yeah?). If so, then we can combine those terms to get:



And then we have, once again,



which is what we *should* get.